Chemistry Cheatsheet

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1. Basics

1.1 Unit conversions

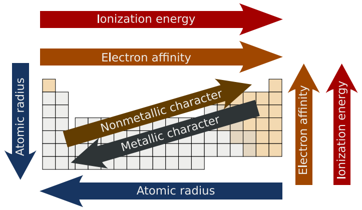
- **Energy:** $1eV = 1.602 \cdot 10^{-19}J$, $1cal = 4.18J$
- **Pressure:** 1Pa=9.892atm=$1.0 \cdot 10^{-5}$bar=$7.5 \cdot 10^{-3}$torr
- **Amount of substance:** 1mol $= 6.022 \cdot 10^{23}$ elementary entities (Avogadro constant)
- **Length:** $1Å = 10^{-10}m$
- **STP thermodynamics:** $25C = 298K$, 1bar, 1mol, 1 cal
- **STP electrochemistry:** $25C = 298K$, 1atm, concentration 1M

1.2 General

- **Kinetic energy:** $E_{kin} = \frac{1}{2} \cdot m \cdot v^2$
- **Potential energy:** $E_{pot} = m \cdot g \cdot \Delta h$
- **electrostatic:** $E_{el} = \frac{\kappa Q_1 Q_2}{d^3}$ $\quad \kappa = \frac{1}{4\pi\epsilon_0}$
- **Photon energy:** $E_\gamma = h \cdot f = \frac{h \cdot c}{\lambda}$
- **De Broglie wavelength:** $\lambda = \frac{h}{m \cdot v}$
- **Specific heat capacity:** $C_s = \frac{q}{m \cdot \Delta T}$

1.3 Trends in the periodic table of elements

- **Ionisation energy:** The ionization energy is the quantity of energy that an isolated, gaseous atom in the ground electronic state must absorb to discharge an electron, resulting in a cation.
- **Electron affinity:** Electron affinity is defined as the change in energy (in kJ/mole) of a neutral atom (in the gaseous phase) when an electron is added to the atom to form a negative ion.
- **Electronnegativity:** Electronegativity is a measure of an atom's ability to attract shared electrons to itself.



2. Atoms

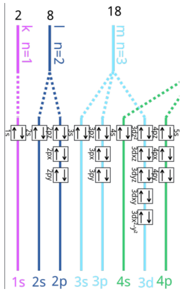
2.1 Quantum mechanics

- Atomic number = #protons = #electrons
- mass number = #protons + #neutrons

Heisenbergs uncertainty principle $\Delta x \cdot \Delta p \geq \frac{h}{4 \cdot \pi}$ Due to duality of electrons (acting like waves and elementary entities at the same time), impossible to exactly describe position and momentum simultaneously.
Effective nuclear charge (approx.): $Z_{eff} = Z - S$
Z = #protons, $S = \#e^-$ on all full shells

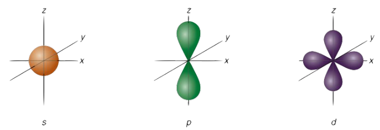
In periodic table: Z_{eff} increases from left to right $\rightarrow$ electrons are more attracted and hence atomic radius is smaller, the further right in the periodic table.

2.2 Orbitals



n	l	subshell designation	m_l	m_s
1	0, s	1s	0	$\pm 1/2$
2	0, s	2s	0	$\pm 1/2$
	1, p	2p	1, 0, -1	$\pm 1/2$
3	0, s	3s	0	$\pm 1/2$
	1, p	3p	1, 0, -1	$\pm 1/2$
	2, d	3d	2, 1, 0, -1, -2	$\pm 1/2$
4	0, s	4s	0	$\pm 1/2$
	1, p	4p	1, 0, -1	$\pm 1/2$
	2, d	4d	2, 1, 0, -1, -2	$\pm 1/2$
	3, f	4f	3, 2, 1, 0, -1, -2, -3	$\pm 1/2$

- **n**: principal quantum number $\rightarrow$ size of orbital
- **l**: angular quantum number $\rightarrow$ shape of orbital
- m_l: magnetic quantum number $\rightarrow$ orientation of orbital
- m_s: spin quantum number



Pauli Exclusion: Each electron has unique set of quantum numbers
Hund's rule: **Every** orbital in sublevel is first singly occupied

3. Chemical bondings

3.1 Covalent bondings

Two atoms share electron pairs
octet rule: Atom tries to acquire noble state (2 valence electrons for H and He, 8 valence electrons for all other)
exceptions:

- Odd electrons
- Less / more than 8 VE's on central atom

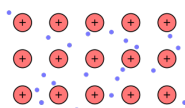
Lewis structure

- Write symbols and connect with single bonds
- Complete ocets around non-central atoms
- Place remaining VE around central atom
- Try multiple bonds if central atom does not have octet
- if multiple lewis structures possible: choose most stable according to formal charge

3.2 Ionic bonding

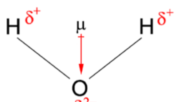
Electrons transfered from atoms with lower EN to atoms with higher EN $\rightarrow$ cations (+) (smaller radius) and anions (-) (bigger radius). electrostatic attraction. $\Delta EN > 1.7 \rightarrow$ ionic bonding
lattice energy ΔU: Energy required to separate ions to infinite distance

3.3 Metallic bonding



cores form grid structure, electron cloud (reason for electricity and heat conduction) surrounds atomic cores

3.4 Polarity and Dipole moment



$\Delta EN > 0.5$: polar bonding, density of e^- higher at δ^- atom. If molecular structure leads to $\rightarrow$ dipole moment exists.

3.5 Formal charges

results if new bondings are formed to satisfy octet rule, ignores electronegativity
Determine formal charge in Molecule:

- split all bondings in middle
- atoms formal charge = VE if unpaired $-e^-$ of that atom after splitting bondings
- effective charge of molecule = sum of formal charges

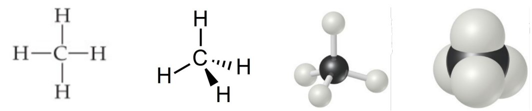
3.6 Bonding strength and length

length: $\equiv < = < -$ **strength:** $- < = < \equiv$

Most stable molecule:

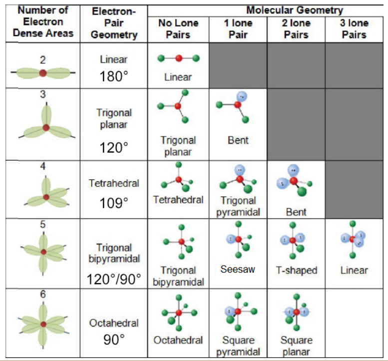
- least formal charges.
- if formal charges necessary: option with the smallest effective charge of molecule
- negative formal charge on electronegative atom

4. Molecular models



structural perspective ball-and-stick space-filling

4.1 valence shell electron pair repulsion (VSEPR)



Number of Electron Dense Areas	Electron-Pair Geometry	Molecular Geometry: No Lone Pairs	1 lone Pair	2 lone Pairs	3 lone Pairs
2	Linear 180°	Linear			
3	Trigonal planar 120°	Trigonal planar	Bent		
4	Tetrahedral 109°	Tetrahedral	Trigonal pyramidal	Bent	
5	Trigonal bipyramidal 120°/90°	Trigonal bipyramidal	Seesaw	T-shaped	Linear
6	Octahedral 90°	Octahedral	Square pyramidal	Square planar	

5. State of matter

5.1 Intermolecular forces

1. **Van-der-Waals interactions** (weak)
   (a) **Dipol-Dipol**
   Sum of all dipole moments from polar bonds in molecule. (molecular dipole) ($\Delta EN > 0.5$)
   (b) **Dispersion**
   Temporary fluctuations of the electrons can cause an induced dipole. **These forces always exist**. Force increases with molecule size and also affected by molecular shape.
2. **Ion-Dipole Interactions** (strong)
   Very important for solutions. Ions solvated by polar liquid.
3. **Hydrogen bonding** (strong)
   One type of dipole-dipole interaction. N, O, F are very electronegativ $\Rightarrow$ very polar bonds with H.

Ion-Dipole > 50kJ/mol $>$ H-Bonding ~ 25kJ/mol $>$ Dipole-Dipole $\approx$ Dispersion ~ 50kJ/s

5.2 Fluids

Colligative Properties: Changes depend on amount of solute added, but not which solute.

Boiling-Point Elevation:

$$\Delta T_b = T_b(\text{solution}) - T_b(\text{solvent}) = iK_b m$$

m = molality of solute
K_b = molal bp elevation constant
i = van't Hoff factor
= 1 for non-electrolytes
= Number of ions produced for electrolytes. e.g 2 for NaCl

Vapor-Pressure Lowering:

$$\boxed{P_{\text{vap}}^{\text{sol}} = X_{\text{solvent}} * P_{\text{vap}}^{\text{pure}}}$$

Raoult's law — Solution is an ideal solution. All intermolecular interactions are identical.

Freezing-Point Depression:

$$\Delta T_f = T_f(solution) - T_f(solvent) = -iK_f m$$

m = molality of solute
K_f = molal fp depression constant
i = van't Hoff factor

5.3 Expressions for Solutions

- X Mole fraction $= \frac{\text{moles solute}}{\text{total moles}}$
- M Molarity $= \frac{\text{moles solute}}{\text{litres solution}}$
- m Molality $= \frac{\text{moles solute}}{\text{kg solvent}}$
- Mass% $= \frac{\text{mas solute}}{\text{total mass}} \cdot 10^2$, ppm: $\cdot 10^6$, ppb: $\cdot 10^9$

5.4 Ideal Gas

- Assumptions of IGL
  - Gas molecules don't occupy much of total volume.
  - Gas molecules don't interact.
- Ideal Gas Law: $pV = nRT = NkT$
- $p\,[Pa]$, $V\,[m^3]$, n [num of moles], $R\,[\frac{J}{mol*K}]$, $T\,[K]$
- Density $\rho = M\frac{n}{V} = M\frac{p}{RT}$

Partial pressure:

$$\boxed{p_i = n_i \cdot \frac{RT}{V} \text{ total pressure} = \sum \text{ of all partial pressures.}}$$

5.5 Osmotic pressure

Pressure needed to counteract osmotic flow.

$$\boxed{\Pi = i\left(\frac{n}{V}\right)RT = iMRT}$$

6. Thermodynamics

6.1 System types

- **Open** Can echange matter and energy w/ surrounding
- **Closed** Can echange energy w/ surrounding
- **Isolated** Nothing can be exchanged

6.2 E = Internal energy of system

- $\Delta E = E_{\text{final}} - E_{\text{initial}}$
  $\Delta E > 0$ system gained energy
  $\Delta E < 0$ system lost energy
- **1st Law of Thermodynamics**
  $\Delta E = q + w$
  q = heat added to system, w = work done on system

6.3 Enthalpy, H

ΔH tells us about heat transferred during chemical reaction.

- $\Delta H = q_p$ heat flow at constant P
- $-P\Delta V =$ pressure-volume work
- $\Delta H > 0 \Rightarrow$ endothermic
  $\Delta H < 0 \Rightarrow$ exothermic

6.4 Heat Capacity

Heat flow required to raise substance's T by 1 degree $^\circ C$ (or K)

$$C_m = \text{molar heat capacity} = \left[\frac{J}{mol * {}^\circ C}\right] = \left[\frac{J}{mol * K}\right]$$

$$C_s = \text{specific heat capacity} = \left[\frac{J}{g * {}^\circ C}\right] = \left[\frac{J}{g * K}\right]$$

$$q = n * C_{m/s} * \Delta T$$

Hess's Law: $\Delta H_{\text{rxn}} = \sum \Delta H_i$
e.g Enthalpies of Formation: ΔH_f°

6.5 Entropy, S

Entropy is a measure of disorder in a system. All spontaneous processes are irreversible. S is a state function.

- $\Delta S = \frac{q_{\text{rev}}}{T}$, $q_{\text{rev}} =$ heat flow for reversible process
- $S = k_b * ln(W)$, $k_b =$ Boltzmann's constant, $W =$ num of microstates

$\boldsymbol{\Delta S > 0}$: increasing microstates
e.g increasing V, increasing T, increasing n, increasing complexity of molecules, melting solids, vaporizing liquids

6.6 2nd Law of Thermodynamics

Entropy of the universe increases for any spontaneous process.

$$\Delta S_{\text{univ}} = \Delta S_{\text{sys}} + \Delta S_{\text{surr}} > 0 \text{ (spontaneous, irreversible)}$$

$$\Delta S_{\text{univ}} = \Delta S_{\text{sys}} + \Delta S_{\text{surr}} < 0 \text{ (nonspontaneous)}$$

$$\Delta S_{\text{univ}} = \Delta S_{\text{sys}} + \Delta S_{\text{surr}} = 0 \text{ (reversible)}$$

6.7 Gibbs Free Energy

$$\boxed{G = H_{\text{sys}} - TS_{\text{sys}} \text{ at constant T}}$$

ΔH	ΔS	$-T\Delta S$	ΔG	Reaction Characteristics
-	+	-	-	at all T Spontaneous
+	-	+	+	at all T Nonspontaneous
-	-	+	+or-	$\downarrow$T Spon.; $\uparrow$T Nonspon.
+	+	-	+or-	$\downarrow$T Nonspon.; $\uparrow$T Spon.

7. Kinetics

7.1 Reaction rate

Given general rxn: $\alpha A + \beta B \longrightarrow \gamma C + \delta D$

$$0 < \text{Rate} = \underbrace{-\frac{1}{\alpha}\frac{d[A]}{dt} = -\frac{1}{\beta}\frac{d[B]}{dt}}_{\text{Rate of disappearance of reactants}} = \underbrace{\frac{1}{\gamma}\frac{d[C]}{dt} = \frac{1}{\delta}\frac{d[D]}{dt}}_{\text{Rate of appearance of products}}$$

7.2 Rate Law

$$\boxed{\text{Rate}[\frac{M}{s}] = k[A]^m[B]^n}$$

- rate only depends on reactants
- k is the rate constant
- m, n are the reaction orders
- m, n can be $0, \frac{1}{2}, 1, 2, \ldots$
- $m + n$ is overall rxn order
- m, n are not necessarily equal to α, β

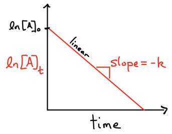
7.3 Reaction Orders

Consider $A \longrightarrow B$
$[A]_t =$ concentration of A at time t
$[A]_0 =$ concentration of A at time $t = 0$

1st Order

$$\text{Rate} = -\frac{d[A]}{dt} = k[A]^1$$

$$ln[A]_t = -kt + ln[A]_0$$

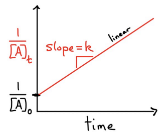


2nd Order

$$[A]_t = [A]_0 exp(-kt)$$

$$\text{Rate} = -\frac{d[A]}{dt} = k[A]^2$$

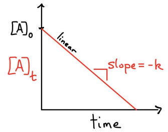
$$\frac{1}{[A]_t} = kt + \frac{1}{[A]_0}$$



Zero Order

$$\text{Rate} = -\frac{d[A]}{dt} = k[A]^0 = k$$

$$[A]_t = -kt + [A]_0$$



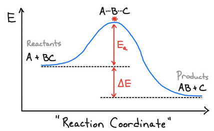
7.4 Half Life

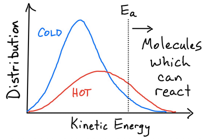
Time needed for $[A]_t = \frac{1}{2}[A]_0$

$$\boxed{\underbrace{t_{\frac{1}{2}} = \frac{0.693}{k}}_{\text{1st Order}} \quad \underbrace{t_{\frac{1}{2}} = \frac{1}{k[A]_0}}_{\text{2nd Order}} \quad \underbrace{t_{\frac{1}{2}} = \frac{[A]_0}{2k}}_{\text{Zero Order}}}$$

7.5 Collision Model

Reaction requires reactant molecules to collide with correct orientation and enough energy.
Higher T: reactants collide more often and with more kinetic E.
Arrhenius
Molecules need minimum energy to react; Activation Energy, E_a





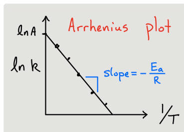
7.6 Arrhenius Equation

$\alpha A + \beta B + \gamma C \longrightarrow$ products
Rate $= k[A]^m[B]^n[C]^p$

$$k(T) = \underbrace{(\tfrac{\text{collisions}}{\text{per time}}) * (\tfrac{\text{fraction of collisions}}{\text{properly oriented}})}_{A} * \underbrace{(\tfrac{\text{fraction of molecules}}{\text{with } E > E_a})}_{* \, exp[\frac{-E_a}{RT}]}$$

A is a "frequency factor", assumed T-independent

$$ln(k) = \frac{-E_a}{R}\frac{1}{T} + ln(A)$$



7.7 Reaction Mechanisms

A sequence of elementary rxns that sum to the overall rxn. The kinetics of elementary rxns are determined by how many molecules have to collide, referred to as the molecularity.

Elementary rxns have rate law where $m, n, p \ldots$ are equal to stoichiometric coefficients.

Molecularity	Elementary rxn	Rate law
Unimolecular	$A \longrightarrow P$	$k[A]$
Bimolecular	$A + A \longrightarrow P$	$k[A]^2$
Bimolecular	$A + B \longrightarrow P$	$k[A][B]$

Multistep Reactions

Overall rate law results from the individual rate laws for the individual elementary reactions.

$$\left.\begin{array}{l} 2A \xrightarrow{k_1} I + C \\ I + B \xrightarrow{k_2} A + D \end{array}\right\} \text{elementary rxns}$$

$$A + B \longrightarrow C + D \; \} \text{ overall rxn}$$

Assume $k_1 << k_2$, i.e. step 1 is "rate limiting"
$\Longrightarrow$ rate overall $= k_1[A]^2$

7.9 Catalysts

Substances that increase rxn rate, but are neither produced nor consumed in overall rxn.

Can $\left\{ \begin{array}{ll} \text{increase A} & \Rightarrow \text{better orient molecules} \\ \text{lower A} & \Rightarrow \text{lower energy of transition state or allow new mechanism} \end{array} \right.$

Lower E_a has bigger impact
$\Rightarrow$ Appears in exponent of $k(T) = A * exp(\frac{-E_a}{RT})$

8. Chemical Equilibrium

$A \underset{k_r}{\overset{k_f}{\rightleftharpoons}} B$, at equilibrium: Rate $= k_f[A] = k_r[B]$

8.1 Law of mass action, equilibrium-constant

molarity concentrations: $K_c = \frac{[C]^\gamma[D]^\delta}{[A]^\alpha[B]^\beta}$

partial pressures: $K_p = \frac{[P_C]^\gamma[P_D]^\delta}{[P_A]^\alpha[P_B]^\beta} = K_c(RT)^{\Delta n}$

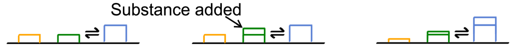
$K >> 1 \rightarrow$ products dominate, $K << 1 \rightarrow$ reactants dominate
K depends on T and is unitless
heterogeneous equilibria: exclude pure solids / liquids from K
reaction quotient Q **if not at equilibrium**, calculated like K_c

- rxn written in reverse: $K = K_{\text{original}}^{-1}$
- rxn multiplied by n: $K = (K_{\text{original}})^n$
- multistep rxn: $K = K_1 \cdot K_2 \cdot K_3 \ldots$
- With catalysts: equilibrium is reached faster, K unchanged

8.2 Le Châteliers principle

Disturbance in concentration
system reacts to consume added substance

Substance added



Disturbance in pressure
reduced volume $\rightarrow$ system shifts in direction with fewer moles of gas
Disturbance in temperature

	Endothermic	**Exothermic**
increased T	right shift	left shift
decreased T	left shift	right shift

9. Acid Base Reactions

9.1 Brownsted Lowry acids and bases

$$\underbrace{HA(aq)}_{\text{acid } (H^+\text{-donor})} + \underbrace{B(aq)}_{\text{base } (H^+\text{-acceptor})} \rightleftharpoons \underbrace{A^-(aq)}_{\text{conjugate base}} + \underbrace{HB^+(aq)}_{\text{conjugate acid}}$$

strong acids/bases completely ionize, weak acids/bases don't

9.2 Autoionisation of water

Amphiprotic substances (ex. Water) can act as acid **and** base

$$\underbrace{H_2O(l)}_{\text{acid}} + \underbrace{H_2O(l)}_{\text{base}} \rightleftharpoons \underbrace{OH^-(aq)}_{\text{conjugate base}} + \underbrace{H_3O^+(aq)}_{\text{conjugate acid}}$$

$$K_w \equiv K_C = [OH^-][H_3O+] = 10^{-14}(25^\circ C)$$

9.3 Reaction of acid with water / base with water

acid-dissociation: $K_a \equiv K_C = \frac{[A^-][H_3O^+]}{[HA]}$

base-dissociation: $K_b \equiv K_C = \frac{[HB^+][OH^-]}{[B]}$

9.4 p-Scales

$p(\xi) = -\log(\xi)$ $\quad pH = -\log[H_3O^+]$ $\quad pOH = -\log[OH^-]$
$pH + pOH = 14$ $\quad pH < 7 \rightarrow$ acid $\quad pH > 7 \rightarrow$ base

9.5 common ion effect and Buffers

$CH_3COOH + CH_3COONa \rightarrow$ dissociates to CH_3COO^-

$$HA(aq) + OH^-(aq) \rightleftharpoons A^-(aq) + H_2O(l)$$

$$A^-(aq) + H_3O^+(aq) \rightleftharpoons HA(aq) + H_2O(l)$$

$$[H_3O^+] = K_a\frac{[HA]}{[A^-]} \rightarrow pH_{\text{buffer}} = pK_a + \log(\frac{[base]}{[acid]})$$

For disturbance small relative to $[HA], [A^-] \rightarrow$ small pH change

10. Redox Reactions

10.1 Oxidation Numbers

- Atoms in elemtal form: **0**
- Monoatmic ions: **ionic charge**
- Nonmetals in ionic/molecular compounds: **negative oxidation numbers**

Oxygen: **-2**	(except peroxide ion, O_2^2-, **-1**)
H: **+1**	(except if bonded to metal, **-1**)
F: **-1**	(always)
Cl, Br, I: **-1**	(except if bonded to oxygen)

- Sum of oxidation numbers for atoms in compound equals its net charge

10.2 Energy and Batteries

- Anode(-): where oxidation occurs
- Cathode(+): where reduction occurs
- Anions migrate towards anode. Cations migrate towards cathode.

Electric potential $=$ potential energy difference per unit charge

$$1V = \frac{1.6 * 10^-19J}{1.6 * 10^-19C}$$

$E^\circ_{\text{cell}} \equiv$ Cell voltage at standard conditions
$E^\circ_{\text{red}} \equiv$ Potential energy available if reduced

Cell potential $\Rightarrow E^\circ_{\text{cell}} = E^\circ_{\text{red}}(\text{cathode}) - E^\circ_{\text{red}}(\text{anode})$

10.3 Connection to Gibbs Free Energy

$$\Delta G^\circ = -nFE^\circ_{\text{cell}}$$

$\Delta G^\circ = $ J/mol of rxn
$F =$ Faraday's constant
$= 96'485$C/mol e^-'s
$n =$ unitless number moles of e^-'s transferred in balanced cell rxn

$E^\circ_{\text{cell}} > 0, \Delta G^\circ < 0$
$\Rightarrow$ **Spontaneous!**